CrystalDirect-to-Beam: Opening the shortest path from crystal to data

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CrystalDirect™(CD) is the world's first, fully automated harvesting system in user operation [1]. The CD harvester automatically harvests, cryo-cools and mounts on SPINE compliant sample holders [2L] crystals grown on an ultra-thin film directly compatible with X-ray data collection. Laser photo-ablation is used to harvest one or several crystals at a time from 96 wells vapour diffusion CD plates, with minimal stress and almost no crystal size limitation. Before harvesting, the solution surrounding the crystals is removed to ensure proper vitrification without adding cryo-protectants [2R]. Associated with a FlexED3 robotic cryo-storage unit [3], the CD harvester of the EMBL Grenoble HTX lab allows harvesting 40 crystal per hour without any manual intervention. The Crystallization Information Management System CRIMS (https://htxlab.embl.fr/) allows the remote pre-location of crystals in CD plates and their tracking until data is collected. In tandem with the fully automated ESRF MX beamline MASSIF-1 [4], the system is extensively used to support high throughput fragment screening applications. CD harvesting is also particularly interesting for difficult projects, such as those involving fragile or micro crystals. Beyond filling the automation gap between crystallization and data collection, CrystalDirect opens a new way to supply beamlines with crystals. Here, we will report on CrystalDirect-to-Beam, a proof of concept made at the ESRF/EMBL beamline ID30B, where a CD harvester is directly coupled to a Flex HCD sample changer [3] and MD2S diffractometer [5]. In this setup, crystals pre-located using CRIMS are automatically harvested and mounted on the goniometer of the MD2S for data collection, either at cryogenic temperature or at room temperatures using a humidity control device. Data can be collected manually or automatically, in parallel with the next crystal harvesting. When automatic, data collection relies on the MXPressR workflow [7]: crystals are pre-centred using crystal coordinates provided by the CD harvester, centred using X-rays and data collected after the strategy is defined from characterisation images. The average crystal turnover-time is currently 6 minutes. Providing crystals in plates also minimizes sample handling efforts and costs, and allows on the fly decisions on the best data collection method, cryo-cooled or at room temperature possibility optimized by crystal dehydration [6]. CrystalDirect-to-Beam should offer the shortest path from crystal to data, and could become standard beamline equipment at sites where crystallization facilities are next to synchrotrons. Suitable for serial data collection with micro-crystals, CrystalDirect could also be used to exploit the characteristics of 4th generation synchrotron beams.

References

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